A Priori Testing of Turbulent Mixing Models for Subgrid-scale Mixing and Reaction *

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Using the data obtained from direct numerical simulations (DNS), *a priori* testing of turbulent mixing models for large-eddy simulations of non-premixed turbulent combustion have been tested, in particular the IEM (Villermaux and Devillon[1]), the modified Curl (Janicka et al.[2]) and the EMST (Subramaniam and Pope[3]). The DNS is performed for single-step, non-premixed reactions developing in incompressible, isotropic, decaying turbulence where local flame extinction and re-ignition occur (cf. Figs. 1 and 2); the simulation domain is divided into subvolumes for testing. In order to demonstrate the "true" performance of the mixing models, the temporal evolution of the fluid particle positions and the exact value of the mixing frequencies within each subvolume are obtained from the DNS, and are utilized in testing. Comparison of the model predictions with the DNS data shows that the EMST mixing model yields reasonable filtered quantities, such as the filtered temperature and filtered reaction rate, while the IEM and the modified Curl mixing models tend to underestimate the filtered quantities (cf. Figs. 3 and 4).

A priori testing of a new mixing model proposed by the authors (Mitarai et al. [4]) will also be presented. Among other things, this new mixing model accounts for the difference between the mixing of passive and of reactive scalars, while the presently available mixing models do not distinguish between them. Given the Lagrangian time series of the mixture fraction and its dissipation rate, this new model well describes the qualitative behavior of the Lagrangian time series of reactive scalars, and yields accurate quantitative statistics.

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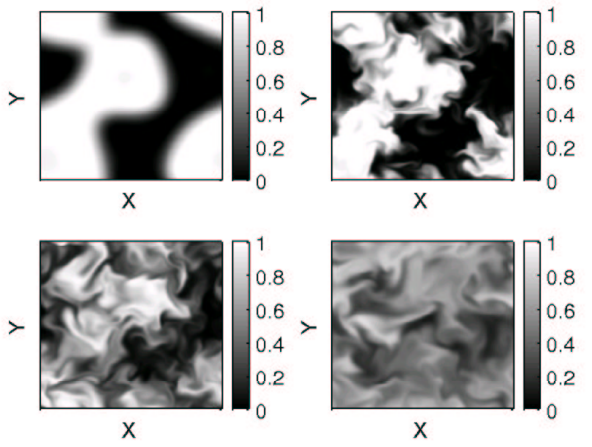

FIG. 1: Temporal evolution of the mixture fraction field on a two dimensional slice through the computational domain.

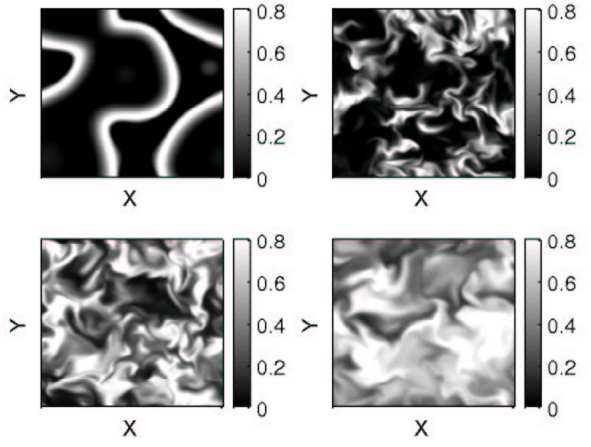

FIG. 2: Temporal evolution of temperature field on the same two dimensional slice through the computational domain as in Fig. 1.

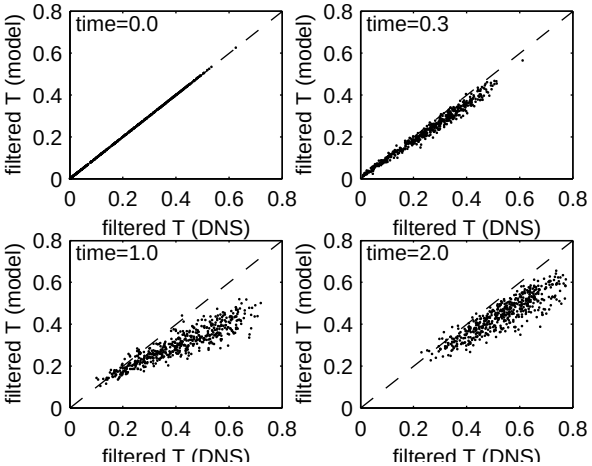

FIG. 3: The filtered temperatures computed from the modified Curl mixing model[2]) plotted against those from the DNS.

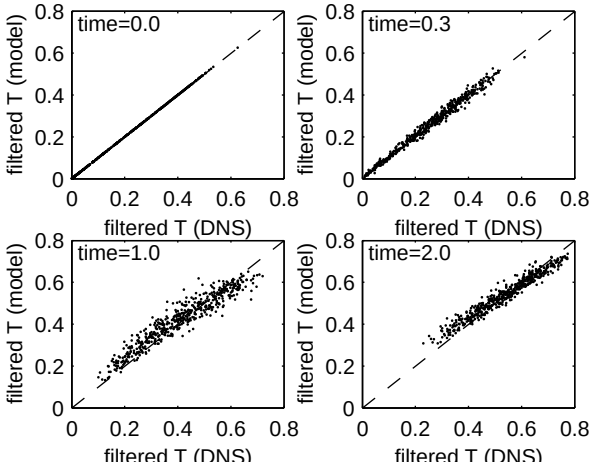

FIG. 4: The filtered reaction rate computed from the EMST mixing model[3] plotted against those from the DNS.

[1] J. Villermaux and J. C. Devillon, in *2nd International Symposia on Chemical Reaction Engineering* (ISCRE, Netherlands, 1972), p. B1.

[2] J. Janicka, W. Kolbe, and W. Kollmann, J. Non-Equilib. Thermodyn. **4**, 47 (1979).

[3] S. Subramaniam and S. B. Pope, Combust. Flame **115**, 487 (1998).

[4] S. Mitarai, G. Kosály, and J. J. Riley (2003), submitted to Combust. Flame.